Photochemical data of stormflow samples collected near Minneapolis and St. Paul, Minnesota from 2014-September to 2015-October

Abstract: Stormflow samples were collected from 31 sites near Minneapolis and St. Paul, Minnesota between 2014-September and 2015-October. Optical and photochemical parameters of the samples were measured under controlled laboratory conditions. The data were collected to better understand the way in which land cover with variable levels of human impact influence the formation rate and yield of triplet excited states of dissolved natural organic matter (^{3}DOM*). Rates of formation ($R_{f,T}$) and apparent quantum yields (AQY_T) were measured for ^{3}DOM* using the chemical probe, 2,4,6-trimethylphenol, under a broadband xenon-arc lamp with a 290-nm wavelength filter.

1. Title of Dataset: Photochemical data of stormflow samples collected near Minneapolis and St. Paul, Minnesota from 2014-September to 2015-October

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3. Data collected: 2014-09 through 2017-03

4. Location of Data Collection:
University of Minnesota
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5. Funding sources:
A. Minnesota Environment and Natural Resources Trust Fund as recommended by the Legislative-Citizen Commission on Minnesota Resources (LCCMR)

B. Doctoral Dissertation Fellowship from the Graduate School at the University of Minnesota
C. National Science Foundation (CBET-143414)

Sharing and Data Access

1. Publication that uses this data:
   McCabe, A. J., and W. A. Arnold (2017), Reactivity of Triplet Excited States of Dissolved Natural Organic Matter in Stormflow from Mixed-Use Watersheds, *Environ. Sci. Technol.*, doi:10.1021/acs.est.7b01914.

   Link: http://pubs.acs.org/articlesonrequest/AOR-yuk8zV83Mp4cYVY5V4vq

2. Suggested citation:
   McCabe, A. J., and Arnold, William A. (2017), Photochemical data of stormflow samples collected near Minneapolis and St. Paul, Minnesota from 2014-September to 2015-October. Retrieved from the Data Repository for the University of Minnesota.

Data Overview

File:
Stormflow_UofMN_Optical_and_Photochemical_Data.xlsx

Description:
This file contains optical and photochemical data measured in stormflow samples from 31 sites near Minneapolis and St. Paul, Minnesota collected between 2014-09 through 2015-October.

Methodological Information

Description of methods used for data collection:
McCabe, A. J., and W. A. Arnold (2017), Reactivity of Triplet Excited States of Dissolved Natural Organic Matter in Stormflow from Mixed-Use Watersheds, *Environ. Sci. Technol.*, doi:10.1021/acs.est.7b01914.

Data-specific information for: Stormflow_UofMN_Optical_and_Photochemical_Data.xlsx

Information for worksheet DOM_Photochem

1. A list of site locations, full names, and cooperating watershed and conservation districts is included at the end of this document.

2. Cell colors of column D are visual indicators of the primary (>20%) watershed land cover for each site.

3. The estimated 95% confidence interval for each variable is reported either in a column adjacent to the data or as a percentage above the respective data.

4. There is one outlier point noted in the spreadsheet, sample ID EK collected on 7-28-15. This sample had a high dissolved organic carbon concentration [DOC] and was excluded from the published analysis.

5. Variable List:
   A. Name: Site ID
      Description: Abbreviated site identification name.
   B. Name: Collection Date
      Description: Date upon which the sample was collected.
   C. Name: Sample Type
      Description: Either Stormflow, Snowmelt, or Baseflow. There are blank rows separating these data groups.
   D. Name: Predominant Watershed Land Cover
      Description: Six characterizations corresponding to the primary (>20 %) of the watershed from which the sample was collected.
   E. Name: Watershed size
      Description: Area in kilometers squared of the watershed from which the sample was collected.
   F. Name: DOC
      Description: DOC is the dissolve organic carbon concentration measured by catalytic combustion [units = mg C L^{-1} and $\times 10^{-4}$ M C].
   G. Name: DIC
      Description: DIC is the dissolved inorganic carbon concentration measured either by alkalinity titration or off-gassed CO_2 after sample acidification [units = mg C L^{-1} and $\times 10^{-4}$ M C].
   H. Name: pH
      Description: pH = -log([H^+]) [unitless].
   I. Name: Specific Conductance
      Description: A measure of the samples ability to conduct an electrical current. A measure of sample's ionic strength [units = µS cm^{-1}].
   J. Name: a254, a350, a440
      Description: These are the absorbance measurements at wavelengths 254 nm, 350 nm, and 440 nm. Absorbance (a) is a ratio measurement over a specific distance, where a = $\log_{10}(I_0/I)$, where I_0 is the incident light intensity and I is the intensity of light after passing through the sample over the specified distance [units = m^{-1}].
   K. Name: E2/E3
      Description: E2/E3 [unitless] is the ratio of the light absorbance of the water sample at a wavelength of 250 nm to the absorbance at 365 nm measured by spectrophotometry.
   L. Name: $SUVA_{254}$
      Description: $SUVA_{254}$ [units = L mg C^{-1} m^{-1}] is the specific ultraviolet (UV) absorbance at the wavelength 254 nm. It is computed as the ratio of the absorbance at

254 nm of the water sample [unitless] to the dissolved organic concentration [units = mg C L^{-1}]. $SUVA_{254}$ is reported in both decadic [log-10] and Naperian [log-e] units.

M. Name: Fluorescence Index (FI)
Description: FI was calculated as the ratio of emission intensities at wavelengths 470 nm and 520 nm at an excitation of wavelength of 370 nm [unitless].

N. Name: Humification Index (HIX)
Description: HIX values were calculated using the following equation:

$$HIX = \frac{\int_{em=435nm}^{480nm} I_{ex=254nm}}{\int_{em=435nm}^{480nm} I_{ex=254nm} + \int_{em=300}^{345} I_{ex=254nm}}$$

Where $I_{ex=254nm}$ represents the emission intensities at an excitation wavelength of 254 nm. HIX quantifies the degree to which emission red-shifts as humification (degradation from biological origin, shifting from low molecular weight bio-labile organics to more condensed aromatics through microbial action) occurs [unitless].

O. Name: Freshness Index (β/α)
Description: β/α was calculated as the ratio of emission intensities at 380 nm (marine- or algal-like, termed β or M components) to the maximum emission intensity between 420 – 435 nm (humic-like DOM, termed α or C components) at an excitation wavelength of 310 nm [unitless].

P. Name: R_a
Description: R_a is the estimated rate of light absorption [units = mol-photons L^{-1} s^{-1}] by the water samples in the solar simulator used throughout this study. R_a was estimated by chemical actinometry.

Q. Name: $[TMP]_0$
Description: The initial concentration of 2,4,6-trimethylphenol used to estimate the rate of triplet formation in all collected stormflow samples (μM)

R. Name: $k_{obs,TMP}$
Description: $k_{obs,TMP}$ is the pseudo-first order rate constant for the photo-sensitized loss of 2,4,6-trimethylphenol (TMP) [units = s^{-1}].

S. Name: IF_{est}
Description: The estimated inhabitation factor for the inhibition of ^{3}DOM*-sensitized photolysis by DOC. All measurements that have been corrected for this inhibition have the superscript, *corr* [unitless].

T. Name: $R_{f,T}$
Description: The rate of formation of triplet excited states of dissolved natural organic matter as measured by the photosensitized degradation of TMP [units = M s^{-1}].

U. Name: $[^3DOM^*]_{ss}$
Description: $[^3DOM^*]_{ss}$ is the steady-state concentration of triplet excited states of dissolved natural organic matter as determined from the photosensitized loss of TMP in the water samples under simulated sunlight [units = M].

V. Name: AQY_T

Description: The apparent quantum yield for the formation of triplet excited states of dissolved natural organic matter computed as the ratio of the rate of triplet formation to R_a [units = mol mol-photons^{-1}].

W. Name: f_{TMP}
Description: f_{TMP} is the quantum yield coefficient for TMP loss computed as the ratio of $k_{obs,TMP}$ to R_a [units = L mol-photons^{-1}]. In this samples set, it is used as a proxy for the efficiency of formation of triplet excited states of dissolved natural organic matter.

Information for worksheet Dilution_Photobleach

1. Rows 5 – 15 contain data for a series of dilutions of two samples: H2-072815 and ALUM-052615. The original samples were diluted up to a factor of 10 while holding pH, specific conductance, and [DIC] constant. The corresponding optical and photochemical data for each sample and dilution are reported.

2. Rows 17 – 27 contain data for a series of prolonged exposures in a solar simulator of two samples: H2-072815 and ALUM-052615. The original samples were photo-exposed for up to 60 hours. No water chemistry parameters were adjusted following the exposure. The corresponding optical and photochemical data for each sample and dilution are reported.

3. For definitions of the variables, please see the variable list under *Information for worksheet DOM_photochem*.

Site Names, Locations, and Cooperating Watershed/Conservation Districts:

Site ID	Cooperating District[a]	Site Full Name or Site Description	Site Coordinates (World Geodetic System 1984)
BELT	RWMWD	Beltline	-93.0414, 44.9473
KC	RWMWD	Kohlman Creek	-93.0468, 45.0265
TBO	CRWD	Trout Brook Outlet	-93.0818, 44.9571
FC	RWMWD	Fish Creek	-93.0088, 44.8977
ALUM	RWMWD	Alum Plant Inlet	-92.9821, 44.9588
EK	CRWD	East Kittsondale	-93.1448, 44.9319
TBEB	CRWD	Trout Brook East Branch at Interstate-35E	-93.0900, 44.9776
COMO3	CRWD	Como 3	-93.1433, 44.9778
MALL	RWMWD	Mall-Schmitt	-93.0194, 45.0331
VPO	CRWD	Villa Park Outlet	-93.1184, 45.0002
STS3P	PLSLWD	Fish Point Park at Fish Point Park Rd	-93.4103,44.7304
R5	RCWD	Rice Creek at CO Road I	-93.1851, 45.1075
C2	RCWD	Clearwater Creek at Centerville Fire Station	-93.0473, 45.1627
OWS10	RCWD	Anoka County Ditch 10-22-32 at Lake Dr	-93.1159, 45.1761
BCDIV	WCD	Brown's Creek Diversion Structure	-92.8457, 45.0697
LC	WCD	Little Comfort Inlet	-92.9322, 45.3124
OC	WCD	O'Conners Creek	-92.7975, 44.8345
FCCD2	PLSLWD	FeCl station Hwy13	-93.4942, 44.6886
TBAA	WCD	Trout Brook at Afton Alps	-92.7782, 44.8571
ST14	PLSLWD	Buck Lake creek at Pandora Rd	-93.4742, 44.6851
ST5B	PLSLWD	Agriculture Ditch at Xeon Ave	-93.5163, 44.6604
CSI13	MCWD	Six Mile Creek Turbid Outlet	-93.7102, 44.8554
ST19	PLSLWD	Agriculture Ditch at Marschall Rd	-93.5007, 44.6921
H2	RCWD	Hardwood Creek at 20th Ave	-93.0404, 45.2001
JD1	RCWD	Ramsey-Washington Judicial Ditch 1 at Hugo Road (JD1.1)	-93.0000, 45.1093
CSI05	MCWD	Six Mile Creek Auburn Inlet	-93.6743, 44.8611
BC15	WCD	Brown's Creek at Hwy 15	-92.8457, 45.0697
CMH06	MCWD	Minnehaha Creek Hiawatha Ave	-93.2127, 44.9154
CMH19	MCWD	Minnehaha Creek Minnetonka Blvd/I494	-93.4550, 44.9412
CMH07	MCWD	Minnehaha Creek Grays Bay Dam	-93.4870, 44.9532
CSI12	MCWD	Six Mile Creek Wassermann Outlet	-93.6795, 44.8461

[a]RWMWD=Ramsey-Washington Metro Watershed District; CRWD=Capitol Region Watershed District; PLSLWD=Prior Lake-Spring Lake Watershed District; RCWD=Rice Creek Watershed District; WCD=Washington Conservation District; MCWD=Minnehaha Creek Watershed District.

Watershed and Conservation Districts may be reached through these webpages:

Ramsey-Washington Metro Watershed District:	www.rwmwd.org
Capitol Region Watershed District:	www.capitolregionwd.org
Prior Lake-Spring Lake Watershed District:	www.plslwd.org
Rice Creek Watershed District:	www.ricecreek.org
Washington Conservation District:	www.mnwcd.org
Minnehaha Creek Watershed District:	www.minnehahacreek.org